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PEACH FRUIT QUALITY ANALYSIS IN RELATION TO ORGANIC AND  
CONVENTIONAL CULTIVATION TECHNIQUES

by

Varun Chandra Koneru

A thesis submitted in partial fulfillment  
of the requirements for the degree

of

MASTER OF SCIENCE

in

Nutrition, Dietetics and Food Sciences

Approved:

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UTAH STATE UNIVERSITY  
Logan, Utah

2013

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## ABSTRACT

Peach Fruit Quality Analysis in Relation to Organic and Conventional  
Cultivation Techniques

by

Varun Chandra Koneru, Master of Science

Utah State University, 2013

Major Professor: Dr. Robert E. Ward

Department: Nutrition, Dietetics, and Food Sciences

The USA is the third major world producer of peaches but consumption has decreased over the last two decades. Consumers have cited mealy texture, fruit browning, and lack of sweetness as some undesirable characteristics in peaches, which may be related to the decline. The focus of this study was to evaluate the effect of farm management practices on fruit quality. The experiment was a completely randomized block design with 10 replicates, three treatments (organic, conventional and transitional organic), and two to four sampling dates as repeated measures. A non-targeted approach based on HS-SPME-GC-MS was used to analyze the volatile compounds in the treatments. Eighty volatiles (alcohols, ketones, aldehydes, esters, lactones, carboxylic acids, phenolics and terpenoids) were quantified and many of these were found to be correlated with the physical parameters of the peaches. Sensory evaluation indicated transitional organic peaches were liked the best and organically grown peaches were least liked. All the treatments were significantly different from each other and consumers preferred the aroma of conventionally grown peaches. There was no statistically significant difference in flesh firmness between the treatments; conventionally grown peaches were larger ( $86 \pm 4$  mm) and were statistically different from transitional organic

( $82 \pm 4$  mm) and organic peaches ( $80 \pm 5$  mm). The titratable acidity to soluble solids content (TA: SSC) ratio of transitional organic ( $14 \pm 1$ ) was statistically significant from conventionally grown peaches ( $11 \pm 1$ ) and organic peaches ( $11 \pm 1$ ). The total phenolic content was found to be significantly higher in transitional organic and organic peaches compared to conventional peaches. Transitional organic fruit were somewhat nitrogen stressed as synthetic N administration was ceased and it may take some time before organic nitrogen builds in the soil. Lower nitrogen composition was associated with greater sweetness, higher polyphenolic defense compounds, and higher dry matter, which may have contributed to the highest liking of the transitional organic peaches during the sensory analysis. Overall, transitional organic peaches were found to have highest SSC: TA, which may affect the overall liking of the fruit, whereas the size of conventional peaches was presumably higher due to the availability of inorganic NPK as fertilizers. Farm management techniques can influence the peach fruit quality and volatile compounds development in the fruits, which can influence the consumer's preference.

(66 pages)

## PUBLIC ABSTRACT

Peach Fruit Quality Analysis in Relation to Organic and Conventional  
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The USA is the third major world producer of peaches but consumption has decreased over the last two decades. Consumers have cited mealy texture, fruit browning and lack of sweetness as some undesirable characteristics in peaches, which may be related to the decline. The focus of this study was to evaluate the effect of farm management practices on fruit quality. Physical parameters (color, firmness and size), volatiles and metabolite data was collected.

Sensory evaluation indicated transitional organic peaches were liked the best and organically grown peaches were least liked. All the treatments were significantly different from each other and consumers preferred the aroma of conventionally grown peaches. Firmness and sugar content of the treatments were not different from each other. The total phenolic content was found to be significantly higher in transitional organic and organic peaches compared to conventional peaches. Transitional organic peaches were more liked and organic were least liked, but the nutritional values in organic peaches can be the point of interest for the consumers.

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## LIST OF SYMBOLS, ABBREVIATIONS AND DEFINITIONS

SPME	Solid Phase Micro-Extraction
HS	Headspace
SSC	Soluble Solid Concentration
NPK	Nitrogen Phosphorus Potassium
GC-MS	Gas Chromatography- Mass Spectrometry
PCA	Principal Component Analysis
TA	Titrateable Acidity
N	Nitrogen
P	Phosphorus
K	Potassium
DNA	Deoxyribo Nucleic Acid
RNA	Ribo Nucleic Acid
ADP	Adenosine Diphosphate
ATP	Adenosine Triphosphate
AMDIS	Automated Mass Spectral Deconvolution and Identification System
NIST	National Institute of Standards and Technology

## INTRODUCTION

The demand for organic foods continues to increase rapidly worldwide (Lester, 2006). By legal definition, traditional organic farming eliminates the use of synthetic fertilizers and pesticides, relies on animal manures, green manures like uprooted crops plowed into soil, off-farm organic wastes to maintain soil fertility, and uses biological and cultural methods to control weeds and pathogens (Browne, Harris, Hofny-Collins, Pasiecznik, & Wallace, 2000). Organic livestock are fed with 100% organically grown feed that is free of pesticides and animal by-products. Organic livestock has to be provided with access to the outdoors, direct sunlight, fresh air and freedom of movement (Smith-Spangler et al., 2012). All organic foods are processed without irradiation or chemical food additives and are free from genetically modified organisms (Smith-Spangler et al., 2012).

The share of organic agricultural land and the organic foods market are increasing in many countries (Yussefi & Willer, 2007). About 120 countries practice organic agriculture. In 2007 Australia had the highest area of organic agriculture at 11.8 million hectares while the U.S had about 1.6 million hectares (Yussefi & Willer, 2007). The U.S organic food and beverage market has grown from \$1 billion in 1990 to \$26.7 billion in 2010 according to organic trade association. A growth of 7.7% was observed in sales from 2009 to 2010 (Yussefi & Willer, 2007).

During the last 20 years there has been a growing interest in the quality variations between organic and conventional foods. Searching the term 'organic foods' in PubMed on December 1<sup>st</sup>, 2012 resulted in 923 references whereas there were 354 references in 2002 and 98 in 1992 ([www.ncbi.nlm.nih.gov/pubmed/](http://www.ncbi.nlm.nih.gov/pubmed/)). Organically grown plants have more

total phenols than conventionally grown plants (Hunter et al., 2011). There is better growth and reproduction in animals fed with organic feed compared with those that are fed with conventional feed (Worthington, 1998). However, a meta analysis concluded that there is no strong evidence that organic and conventional foods are different in major nutrients like sugars, vitamins and minerals with the exception of nitrate (Bourn & Prescott, 2002). A second meta analysis analyzed 55 published studies and concluded that conventionally grown crops have a significantly higher nitrogen content whereas organically grown crops contain more phosphorus and a higher titratable acidity (Dangour et al., 2009). While investigating the nutrient difference between organic and conventional foods studies in the above meta analysis (Dangour et al., 2009) have narrowed down their analyses to a small range of components such as protein, sugars, vitamins and minerals (Bourn & Prescott, 2002). However, it is important to investigate the effects on secondary metabolites such as alkaloids, terpenoids, saponins, phytoalexins, phenolic glycosides and others as they are responsible for defense against microorganisms, herbivores and competing plants (Wink, 1988). In addition they are also responsible for nitrogen transport, nitrogen storage and protection against ultraviolet rays (Wink, 1988). The focus of this study is to investigate whether farm management practices, such as organic and conventional farming, affect the fruit quality.

The hypothesis of this study is:

Farm management techniques might affect the peach fruit quality.

The objectives of this thesis are:

1. To investigate the effect of farm management techniques on peach fruit quality.

2. To estimate the clustering and establish a relation between volatile compounds and treatments using principal component analysis (PCA).

## **LITERATURE REVIEW**

### **Farm Management Practices**

Some studies have concluded that consumers believe that organically grown fruits and vegetables are more nutritious, environmentally friendly and safer (Lester, 2006). Agricultural practices may affect fruit composition as plants with resistance to microorganisms and herbivores tend to have high levels of defense-related secondary metabolites (Mitchell et al., 2007). While the obvious divisions between organic and conventional farming rest on the use of synthetic pesticides, use of different forms of nitrogen likely have major effects on fruit and vegetable quality. In conventional farming, farmers utilize synthetic fertilizers to address deficiencies in soil nitrogen that limit production of biomass (Drinkwater, Letourneau, Workneh, Van Bruggen, & Shennan, 1995). In contrast, organic systems emphasize the accumulation of soil organic matter and fertility (including fixed nitrogen) over time through the use of cover crops and manures and depend on the activity of a diverse soil ecosystem to make nitrogen and other nutrients available to plants (Mitchell et al., 2007). In conventional farming, the inorganic nitrogen, phosphorus and potassium (NPK) may influence the synthesis of secondary metabolites, proteins and soluble solids compared to the nitrogen sources used in organic farming. Restriction of fertilizers in organic procedures results in a lower nitrogen content in the fruits when compared to the fruits grown conventionally (Shaver & Chapin, 1995).



## **What is Fruit Quality?**

The quality of fresh fruits results from a combination of physical and biological attributes (Kader, 1999). Consumers judge the quality of the fruits mostly by their appearance, firmness and aroma. Climacteric fruits like peaches, can be ripened off the plant, they are picked mature but unripe so that they can withstand the postharvest handling system during shipment (Kader, 1999). Soluble solid content (SSC) is measured by a refractometer and expressed in degrees brix which is equivalent to percentage of sucrose in the solution. Titratable acidity (TA) is a measure of the total acid concentration in the given solution and for peaches it is expressed as g/100 ml as malic acid equivalents. California's mandatory quality standards for peaches establish a minimum of 11% SSC with a  $TA \leq 0.7\%$ . These parameters are necessary to satisfy 80% of consumers and the SSC: TA ratio is also important in relation to customer acceptance (LaRue & Johnson, 1989). Fruits with 9-13.5 Newton's flesh firmness are considered as "ready to eat" and harvest date is determined when skin ground color (background color of the peach skin) changes from green to red using a color chip guide (LaRue & Johnson, 1989). In general, peaches with a diameter greater than 74 mm are considered to be large and below that are considered to be small (Blasco, Aleixos, & Moltó, 2003). Thus it can be concluded that SSC, TA, SSC: TA, color, firmness and size are readily measurable characteristics that predict the peach fruit quality.

## **Major Nutrients That Effect the Plant Growth**

### **Nitrogen Importance in Plant System**

Nitrogen (N) plays an important role in developing chlorophyll and amino acids. Nitrogen fertilization increases tree N content by increasing organic dry mass and N concentration throughout the plant growth. Plant uptake of N is principally through the root system and is a function of N availability and concentration (Rehman, Farrukh Saleem, Ehsan Safdar, Hussain, & Akhtar, 2011).

Soil microorganisms like bacteria and fungi convert decomposing organic matter which can be converted to ammonia N ( $\text{NH}_4^+$ ) through mineralization (Pidwirn, 2002). Clay particles in the soil adsorb ammonia onto their surface (Simonne, 2003). The positively charged ammonium ion may also associate with negatively charged soil colloids and this method is called micelle fixation. Micelle fixation is reversible and  $\text{NH}_4^+$  may be discharged through cation exchange from the colloids (Pidwirn, 2002). In addition, microbes may convert  $\text{NH}_4^+$  to nitrate ( $\text{NO}_3^-$ ) (Simonne, 2003). Ordinarily  $\text{NO}_3^-$  accumulates in the soil not adsorbed onto the soil colloids but in solution. If  $\text{NO}_3^-$  is not taken up by the plants, it may leach into ground water (Simonne, 2003).

Nitrogen is a distinguishing component of all amino acids and proteins (Mills & Jones, 1996). In addition to its role in protein composition, nitrogen is an integral part of chlorophyll. An adequate supply of N enables vigorous vegetative growth and a dark green color, while imbalances with respect to other nutrients, such as P, K, and S will slow growth and delay crop maturity (Marti & Mills, 1991).

## **Phosphorus**

Phosphorus is the most essential nutrient element after nitrogen. It is a structural element in Deoxyribo nucleic acid (DNA) and Ribo nucleic acid (RNA) which play a vital role in growth and reproduction of living organisms (Schachtman, Reid, & Ayling, 1998). Adenosine diphosphate (ADP) and Adenosine triphosphate (ATP) help to develop internal energy in the living organisms. Improper P supply may result a reduction in RNA synthesis, and depressed growth (Hedley, Stewart, & Chauhan, 1982). Phosphorus-deficient plants are characterized by a restricted root system and thinner stems. Older leaves turn purple in several plants due to the development of anthocyanins (Jones, Dennis, Owen & Van Hee, 2003). In the tropics, soils contain large amounts of iron and aluminum oxides that bind P firmly, making P biologically unavailable (Schachtman, Reid, & Ayling, 1998). Generally phosphorus in all its forms is insoluble and poorly absorbed from soil. Thus, when P is applied in fertilizer or manure it generally is applied in excess to what the crop takes up (Schachtman, Reid, & Ayling, 1998).

## **Potassium**

Crops require large quantities of potassium (K) to maintain the osmotic pressure of cells (Hedley, Stewar, & Chauhan, 1982). K plays a major role in water management within plant since the osmotic potential of cells is regulated by it. K participates in the closure and opening of stomata. Water uptake, retention and transportation within xylem and of photosynthesis within phloem are affected by K levels (Cakmak, 2005). Cell extension is affected by K and with balanced levels of K, plant resistance to pests and disease increases as it thickens the cell walls of the plants. This, in turn, increases the shelf life of fruits and vegetables. Conversely, plants with K deficiency show less

resistance to diseases and their fruits and seed are smaller in size and deformed (Jungk & Claassen, 1986).

### **Fruit Maturity**

As peach fruit gets to the completion of development, the fruit matures and begins to ripen. Maturity refers to complete development and ripening implies readiness to consume (Lester, 2006). Fruit goes through several changes during maturation like a decrease in flesh firmness, a modified color from green to yellow and a significant increase in flavor (Sánchez, Besada, Badenes, Monforte, & Granell, 2012). Throughout maturity and ripening quality parameters change and ripening will increase sugar concentration, and the presence of aromatic compounds, and decrease in acid and the firmness of the fruit (Kader, 1999). For acceptable fruit quality the soluble solids concentration should exceed 10% at harvest (Kader, 1999).

### **Fruit Volatile Compounds**

Fruit aroma is defined by the volatile compounds such as alcohols, aldehydes and organic acids (Sánchez, Besada, Badenes, Monforte, & Granell, 2012). Aroma plays a key role in consumer acceptability (Cevallos-Cevallos, Reyes-De-Corcuera, Etxeberria, Danyluk, & Rodrick, 2009). Volatile component concentration tends to increase with advancing maturity (Sánchez, Besada, Badenes, Monforte, & Granell, 2012). There are large numbers of volatile compounds found in fruits. One effective method to measure them is headspace solid phase micro extraction (HS SPME) with GC-MS. HS SPME is a solvent free sample preparation technique where a silica fiber coated with polymeric

organic liquid is placed on the head space above the sample (Zhang & Pawliszyn, 1993). The volatile analytes are extracted and concentrated on the coating and then transferred to the GC-MS injection port for desorption and analysis. HS SPME is chosen as an extraction method because it is rapid, easy and inexpensive when compared to liquid-liquid extraction or solid-phase extraction (Smith-Spangler, 2012).

### **Metabolomic Analysis of Food**

Metabolomics is the study of the small molecule metabolites through chemical fingerprints that are left behind by the specific cellular processes of the organism (Cevallos-Cevallos, Reyes-De-Corcuera, Etxeberria, Danyluk, & Rodrick, 2009). Metabolomics can be used in food industry in food component analysis, food consumption monitoring, designing new approaches in nutrition, food security and food quality (Wishart, 2008). Metabolomics analysis can be characterized into targeted and untargeted analysis. In targeted analysis, a selected group of metabolites is identified and quantified (Cevallos-Cevallos, Reyes-De-Corcuera, Etxeberria, Danyluk, & Rodrick, 2009). Conversely, an untargeted metabolomic approach gives a wider picture of the metabolite dynamics in food at the expense of quantitation (Cevallos-Cevallos, Reyes-De-Corcuera, Etxeberria, Danyluk, & Rodrick, 2009). The nutritional quality of fruits is correlated with the presence of soluble sugars, organic acids and some major secondary metabolites like volatiles, flavonoids and pigments (Reganold et al., 2010).

## GC-MS

GC-MS is a common method used in metabolomics. GC-MS is a great analytical tool that can be used to measure volatile and semi-volatile compounds. The process involves the separation of chemicals based on their gas volatility and other physical parameters. MS is used to identify the chemicals based on their mass signatures. Chemicals separated in the GC move to MS and are bombarded with electrons causing fragmentation. The charged ions pass through an electromagnetic filter where the ions are separated based on their mass and the detector counts the ions with specific mass and creates a mass spectrum.

In food metabolomics analysis using GC-MS the metabolites are first oximated and subsequently silylated (Wishart, 2008). Condensation of compounds with hydroxyl amine or methoxy amine is oximation and silylation substitutes the hydrogen atom which is bound to a hetero atom by a silyl group forming a silicon bond and thus protects from further alterations of molecule (Hong et al., 2012). Different small polar molecules can be analyzed by GC-MS such as organic acids, sugars, alcohols, aldehydes, amines and acyl monophosphates. This method is popular in metabolomics studies, since every biofluid or food consists of such components (Wishart, 2008). There are large databases of mass spectra as references that aid in the identification of compounds in food samples. Once the samples are passed through the GC-MS and the peaks are recorded, the samples are sent to the Automated Mass Spectral Deconvolution and Identification System (AMDIS) and the components are identified using the libraries from the databases. These results can be manually integrated to detect components using the software program Spectconnect without any need for a reference library or manual interpretation.

## **The Automated Mass Spectral Deconvolution and Identification System**

AMDIS is a freely available software program that extracts data for individual spectra of components that are found in a GC-MS data file. It conducts noise analysis and removal followed by component perception, deconvolution and then compound identification by matching the spectra to the target libraries such as National Institute of Standards and Technology (NIST).

## **SPECTCONNECT**

SpectConnect is a freely available analytical source at <http://spectconnect.mit.edu>. SpectConnect tracks the peaks of known and unknown metabolites across replicates and no reference spectra is required. SpectConnect tracks and compares components between every spectrum in each sample and compares them with the spectra of the other samples. (Stycznski et al., 2007) concluded that the important compounds will be conserved across most or all replicates, while the noise will be eliminated.

## MATERIALS AND METHODS

### Experimental Design

The study design was a completely randomized design with 10 replicates, three treatments, and two to four sampling dates as a repeated measure.

- Treatment 1: Herbicide + Nitrogen, Phosphorus and Potassium NPK (conventional, n = 27).
- Treatment 2: Herbicide + NPK (transitional organic, n = 45; first year in transition to organic).
- Treatment 3: Paper mulch + organic herbicide + compost (organic, n = 10).

Conventionally grown peaches were given triple sixteen NPK along with urea to increase the available nitrogen to the plants. Organically grown fruits were given paper mulch, organic herbicide and compost. Transitional organic trees were established in 2008 and were grown conventionally for four years, then in the fifth year (2012) the trees were given organic herbicide, paper mulch and compost as in the organic treatment. This process leads to nitrogen stress as the trees had become accustomed to available nitrogen from synthetic fertilizers, but subsequently nitrogen needs to develop in the soil from the organic inputs which affects the nitrogen availability.

Peaches were transported from Kaysville Research Farm (Kaysville, UT) to Nutrition Food Science building (Logan, UT) after they were picked at harvest. Fruits were cooled to refrigeration temperature after picking and were processed two days after harvest for consistency.



### **Peach Size Measurement**

Equatorial and top diameter of each peach sample was recorded using a digital Vernier scale (Carrera Precision 5906, La Verne, CA). The scale was calibrated to zero before every reading. Top diameter was measured from the end of the stem to the apex and equatorial diameter was the circumference at the mid portion of the fruit.

### **Pit Size Measurement**

Peaches were cut vertically from both ends to open it in half and then the pit was removed by careful removal of flesh surrounding it. The Vernier scale was used to measure the length and width of the pit. Both pit length and width were recorded for each individual peach.

### **Skin Color Determination**

Color variation was measured on the skin of peaches. Overall, peaches have a lighter shade (spot) near the stem while the remaining surface is darker. Color measurements were taken at both darker and lighter areas for every individual peach using a Hunter calorimeter  $L^*$ ,  $a^*$  and  $b^*$  values were recorded to calculate the hue angle ( $h^0$ ).

### **Flesh Firmness**

Flesh firmness was measured with a TMS Pro texture analyzer (Food Technology Corp, Sterling, VA) with a compressive force was applied using a 50-kg load cell. A partial hemispherical probe (Magness- Taylor type) of 9 mm in diameter was attached to the load cell moving at a speed of 12 cm/min. Flesh firmness was determined by carefully removing the skin at the equatorial cheeks on the both halves without ripping of the flesh and the fruit was placed in a cylindrical ring so that it didnot move while being punctured by the probe. The skins were carefully peeled after the firmness test and flesh samples were cut into thin slices. About 5 g of each sample was stored in 15 ml centrifuge tubes (Fisher Scientific, Denver, CO) at -80 °C for SPME GC-MS volatile analysis.

### **Soluble Solid Content**

Fruit samples were cut and pureed in a blender for 1 min. The resulting slurry was filtered, centrifuged (20 min; 10,000 x g; 4 °C) and the clear supernatant was collected to determine SSC. Remaining supernatant was stored in centrifuge tubes at -80 °C for TA calculation. SSC was measured using a digital refractometer (Hanna, Woonsocket, RI) standardized after every five samples with distilled water to a refractive index 0% SSC.

### **Titrateable Acidity**

Frozen samples were thawed and TA was determined with an automatic titrator (Mettler Toledo, Columbus, OH). Two grams of sample was mixed with 50 ml of deionized water and titrated by 0.1 N sodium hydroxide until pH 8.2 was reached. TA is expressed as percent malic acid equivalents.

### **SPME GC-MS Volatile Analysis**

Volatile sample preparation was carried out as described by Sánchez et al.(2012) with modifications. Frozen peach samples were finely grounded to a powder in liquid nitrogen using a mortar and pestle. Frozen tissue powder (500 mg) was weighed in a 4 ml vial and 500µl of 100 mM EDTA (pH 7.5) solution and 1.1 g of  $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$  were added immediately to restrict enzyme activity. The vial was sonicated and centrifuged at  $300 \times g$  for 3 min. Approximately 1 g of supernatant was then transferred into 20 ml head space vials and incubated at 50 °C with 500 rpm agitation for 10 min. Subsequently volatiles were adsorbed onto a 65 µm poly dimethylsiloxanedivinybenzene fiber (Supelco, St. Louis, MO) and subsequently desorbed in the injection port of a Shimadzu GC-MS (QP 2010S,Kyoto, Japan) for 1 min at 270 °C in splitless mode. Separation was performed on a ZB-5 MSi column (35.0 m length, 0.25 mm diameter and 0.25-µm film thickness). Helium was used as the carrier gas at a flow rate of 1.0 ml/ min. The temperature program started at 60°C for 1 min, followed by a 10°C/min-ramp to 325°C, with a 10-min hold at 325°C.

### **Extraction of Phenols**

The phenols extraction protocol was carried out as described in Luthria et al. (Luthria, Mukhopadhyay, & Krizek, 2006). For each extraction, approximately  $500 \pm 1\text{mg}$  of ground freeze-dried peach sample was placed in a 15ml centrifuge tube with 5 ml of the solvent mixture Methanol: $\text{H}_2\text{O}$  (80:20, % v/v). The vials were then placed in a sonicator bath (New Brunswick Scientific, G76, Edison, NJ) at ambient temperature for 30 minute. The mixture was centrifuged and the supernant collected. The residue was

resuspended in 5 ml of Methanol: H<sub>2</sub>O (80:20, %v/v), gently mixed manually and sonicated for an additional 30 min followed by centrifugation. The supernant was combined with the initial extract and dried under nitrogen at 40 °C. Completely dried sample was taken in 2 ml of extraction solution and assayed by a Folin–Ciocalteu (FC) assay for total phenol (TP) content. For each sample, duplicate extractions and analyses were carried out.

### **Folin–Ciocalteu Assay Protocol**

The FC assay was modified from Luthria et al. (Luthria, Mukhopadhyay, & Krizek, 2006); it was carried out by pipetting 500 µl of peach extract into a 12 ml amber vial. This was followed by addition of 3.5 ml of deionized water. This mixture was vortexed for 10–20 s and 500 µl of FC reagent was added. The mixture was vortexed for an additional 20–30 s and 1.5 ml of 20% sodium carbonate solution was added after the 1<sup>st</sup> min and before 8<sup>th</sup> min of addition of the FC reagent. The mixture was then vortexed for 20–30 s after the last addition of sodium carbonate at 8<sup>th</sup> min and placed in dark. After 2 h±3 min at room temperature, the absorbance of the colored reaction product was measured at 765 nm. A calibration curve was created using different concentrations of standard gallic acid solutions, each time an analysis was run. The level of TP in the extract was calculated from the standard calibration curve. Results were expressed on the basis of mg of Gallic Acid Equivalent per gram (mg GAE/g) of dried peach powder.

### **Metabolites Extraction Protocol**

Metabolites extraction was carried out as described in Roessner-Tunali et al (Roessner-Tunali et al., 2003). Frozen tissue powder (500mg) was weighed in a 15 ml centrifuge tube and 2 ml of methanol was added to extract the metabolites. One hundred micro liters of as internal standard (0.2 mg/ml ribitol) was added to the peach mixture in the 15ml centrifuge tube. The mixture was extracted for 30 min in a 50°C water bath with shaking. Deionized water (1.2) ml was added into the tube and vortexed. Centrifugation was carried out at 2,200xg for 15 min. Supernatant was transferred into a 4 ml plastic tube. The supernatant in the 4 ml tube was frozen with liquid nitrogen, and then lyophilized for 18 hrs at -80°C.

### **Derivitization**

One hundred and twenty micro liters of 15 mg/ml methoxyamine hydrochloride in pyridine was added to the 4 ml plastic tube containing lyophilized samples and incubated at 50°C, and sonicated. One hundred and twenty micro liters (120 µl) of Bis(trimethylsilyl)trifluoroacetamide+ 1% Trimethylchlorosilane was subsequently added and the solution was incubated for 30 min at 50°C. 1.0 µl of the solution was injected at 25:1 split ratio onto a GC equipped with a DB-5-MS (35.0 m length, 0.25 mm diameter and 0.25-µm film thickness) column coupled to a MS. The injection port was held at 280°C, and the oven ramped from 80°C (2 min) to 315°C (6 min) at 5°C/min. The MS source was held at 250°C and the quadropole at 150°C and scanned from 50 - 650 m/z.

## **Statistical Analysis**

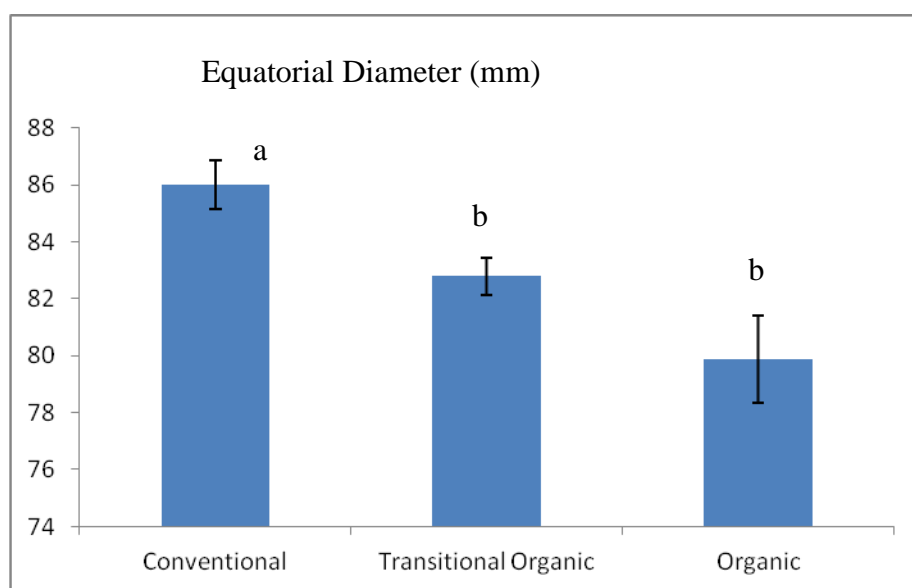
All statistical treatments were performed using IBM SPSS statistics software (v 19, Armonk, NY). The physical parameters and volatiles data were analyzed using one way ANNOVA. Sensory analysis was carried out by Dr. Silvana Martini in the sensory kitchen at Utah State University. Principal component analysis (PCA) was performed using SPSS software to detect clustering and establish a relation between treatments and volatile compounds. Correlation analysis was carried out to determine certain volatiles that might influence the physical parameters between the individual treatments. Data analysis was carried out after the samples were run on GC-MS. Retention Index (RI) data was collected once the n-alkanes were run and RI library was built to correct the retention indices of the analytes. Chromatograms were run on AMDIS using RI calibration data and then submitted to spectconnect. All missing values in volatiles and metabolites data set were replaced by least values in the chromatogram (Xia, Psychogios, Young, & Wishart, 2009).

## RESULTS AND DISCUSSION

### Effect of Treatments on Physical Parameters

#### Size Variance Between the Treatments

The equatorial diameter of the fruits showed that conventionally grown fruits were significantly greater in size ( $p > 0.05$ ) than organic and transitional organic fruits as shown in Figure 1. There was no significant difference observed between the transitional organic and organically grown peaches.



*Figure 1.* Equatorial Diameter of Peaches as a Function of Treatment.

The top diameter of the fruits showed there is no significant difference between the conventional, organic and transitional organically grown fruits as shown in Figure 2. Although organically grown peaches appeared to have a larger top diameter the difference was not significant between treatments (Figure 2). In general peaches with an equatorial diameter greater than 74 mm are considered to be large (Blasco, Aleixos, & Molto, 2003). Peaches grown under these three different treatments were larger than

typical peaches available in market. This might be due to an early frost in 2012 which resulted in fewer fruits per branch.

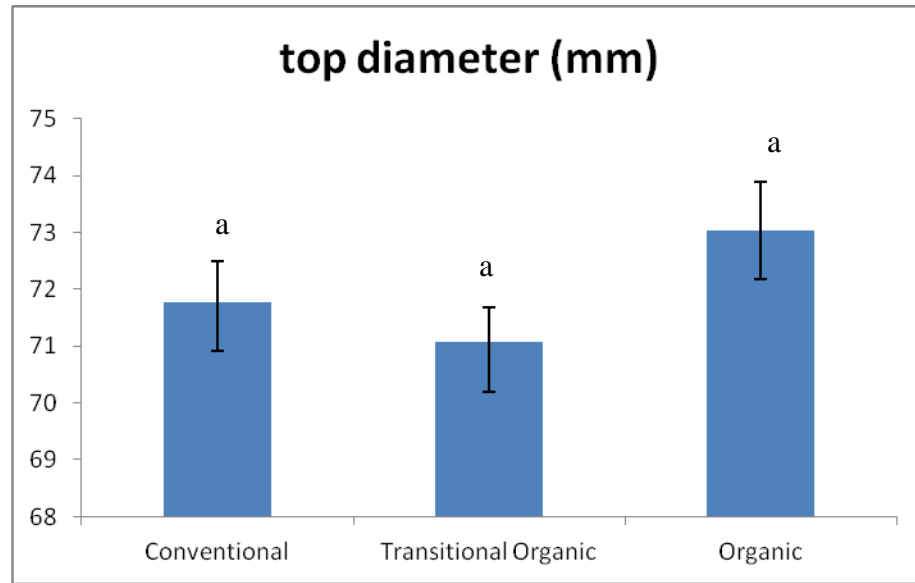


Figure 2. Top Diameter of Peaches as a Function of the Treatment.

Tables 1 and 2 shows there was no significant differences between the pit length and pit width peaches grown under organic, transitional organic, and conventional treatments.

Table 1

*One-way ANOVA for Pit Length as a Function of Treatment*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Organic vs Conventional	0.552	0.603	2.389	0.819	No
Organic vs Transitional organic	0.642	0.742	2.389	0.739	No
Conventional vs Transitional organic	0.090	0.149	2.389	0.988	No



Table 2

*One-way ANOVA for Pit Width as a Function of Treatment*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Conventional vs Transitional organic	0.245	0.647	2.389	0.795	No
Conventional vs Organic	0.356	0.618	2.389	0.811	No
Transitional organic vs Organic	0.111	0.204	2.389	0.977	No

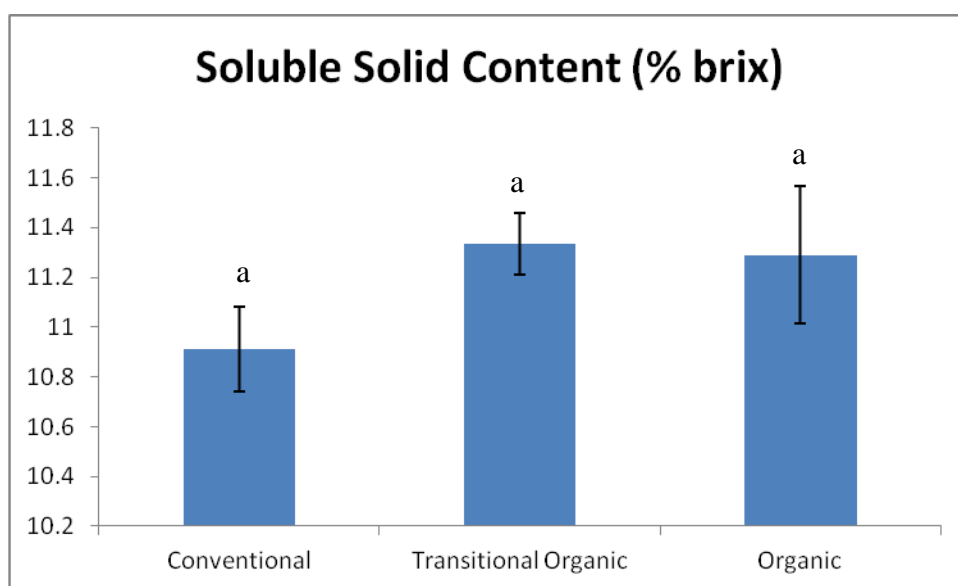
**Peach Fruit Color Variance Between the Treatments**

The overall treatment effect on Hunter color values are shown in Table 3. The redness ( $a^*$ ) and hue angle values of the light spot were significantly affected by the organic treatment when compared to conventional and transitional organic treatments. Color can be quantified by hue angle, where  $0^\circ$  = red,  $90^\circ$  = yellow, and  $180^\circ$  = green. The decrease in hue angle in organic peaches at the light spot can be due to the carotenoid accumulation since decreased carotenoid content has been shown to correlate with a decrease in hue angle (Ruiz, Egea, Tomas-Barberan, & Gil, 2005). On the dark side of the peach fruits there is no significant difference between the  $L^*$ ,  $a^*$ ,  $b^*$  and hue angle.

**Soluble Solids Content**

Figure 3 shows soluble solids content values between the treatments. There was no significant difference observed in SSC between the treatments. This is in agreement with the conclusions of a systematic review of 55 satisfactory quality-crop studies, which concluded that there is no evidence of difference between SSC in organic and conventionally grown fruits (Dangour et al., 2009). All the treatments met with California standards for consumer's acceptance with respect to SSC (LaRue & Johnson, 1989).

Although there was no significant difference in SSC between the treatments the SSC: TA ratio is more closely related to consumer acceptance than SSC alone (Iglesias & Echeverria, 2009). Most of the studies on organic and conventional farming reported there was no significant difference in the SSC but TA acidity tends to show significant difference between the treatments (Dangour et al., 2009). This demonstrates the importance of SSC: TA ratio in consumer acceptability, as sugars and organic acids mostly influence the consumer liking higher the value of SSC: TA gives higher consumer acceptability.

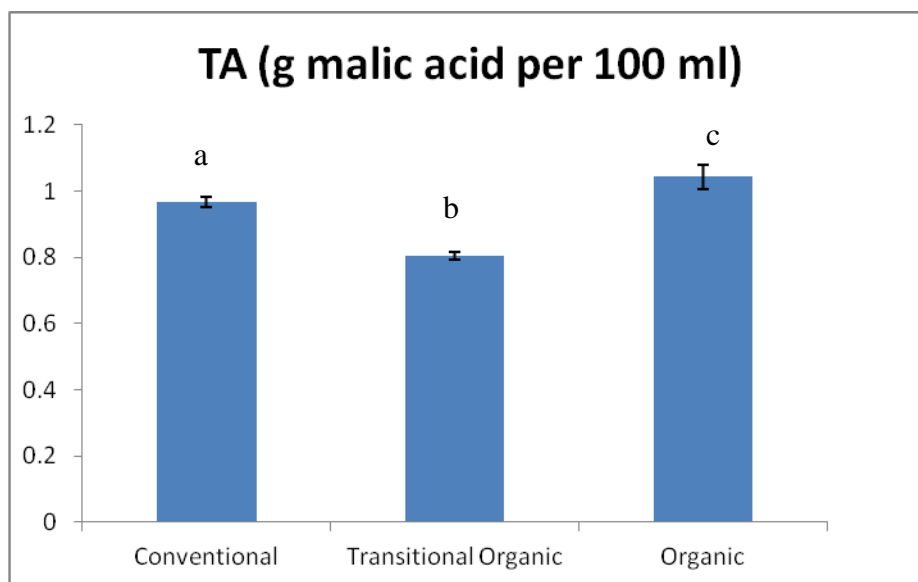


*Figure 3.* Soluble Solid Content of Peaches as a Function of the Treatment

### **Titrateable Acidity**

The titrateable acidity of the peaches grown under conventional, organic and transitional organic treatments showed significant differences between the treatments. Organically grown peaches had higher titrateable acidity followed by conventional and transitional organic peaches had least titrateable acidity (Figure 4).

These results are in agreement with the Dangour et al., 2009. It is also expected that the degree of liking of the peaches is affected by the TA and SSC. As there was no significant difference between the SSC between the treatments, the TA may explain the results from the sensory panel as the lowest degree of liking value was given to the organic peaches which has significantly higher percentage of TA and lower SSC: TA ratio ( $10.9 \pm 1.1$ ).



*Figure 4.* TA of Peaches as a Function of the Treatment.

Table 3

*Hunter color mean values of peaches treated with different treatments*

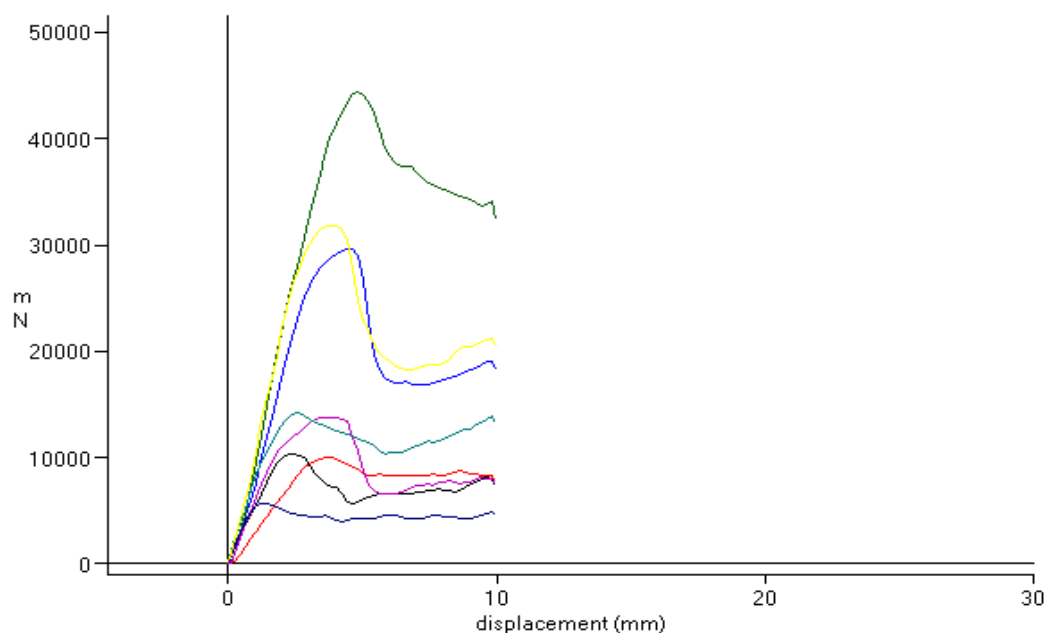
Treatments	Light spot				Dark spot			
	L*	a*	b*	Hue	L*	a*	b*	Hue
Conventional	64±4 <sup>a</sup>	14±4 <sup>a</sup>	36±4 <sup>a</sup>	20±7 <sup>a</sup>	41±4 <sup>a</sup>	19±5 <sup>a</sup>	14±3 <sup>a</sup>	36±5 <sup>a</sup>
Transitional organic	62±6 <sup>a</sup>	15±6 <sup>a</sup>	33±5 <sup>a</sup>	24±10 <sup>a</sup>	40±3 <sup>a</sup>	17±4 <sup>a</sup>	12±2 <sup>a</sup>	39±5 <sup>a</sup>
Organic	61±5 <sup>a</sup>	7±3 <sup>b</sup>	34±4 <sup>a</sup>	12±5 <sup>b</sup>	40±4 <sup>a</sup>	16±6 <sup>a</sup>	12±3 <sup>a</sup>	39±8 <sup>a</sup>
<i>p</i> – value	NS	0.002	NS	0.001	NS	NS	NS	NS

\**p*-value significance at 0.05; NS= not significant; values within column sharing letters (a,b) are not significantly different; Values are mean±SEM

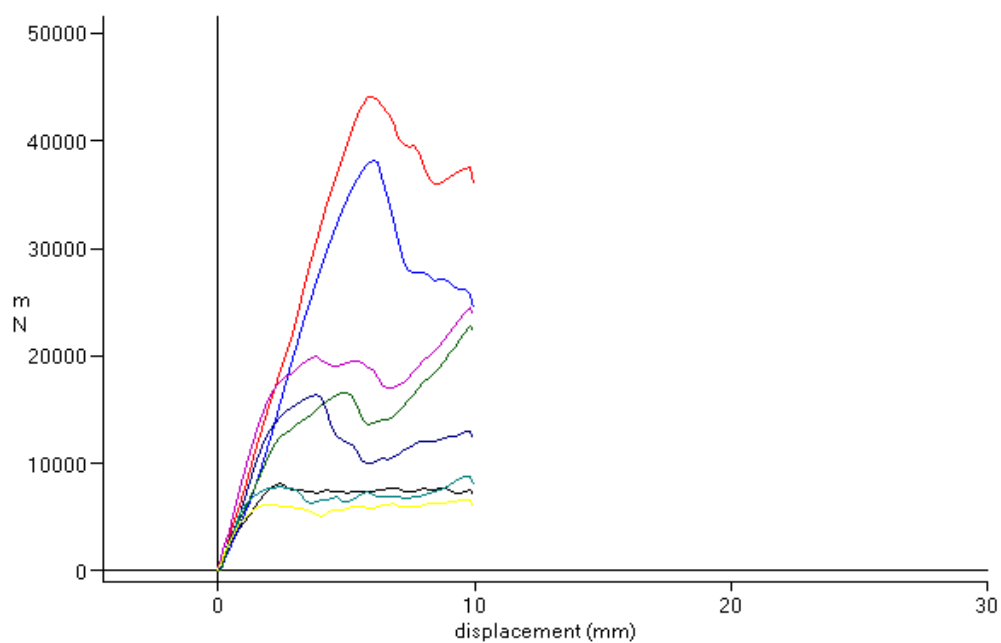
L\* = lightness; a\*= redness; b\* = yellowness; hue angle =  $\text{atan}(b^*/a^*)$

## Firmness

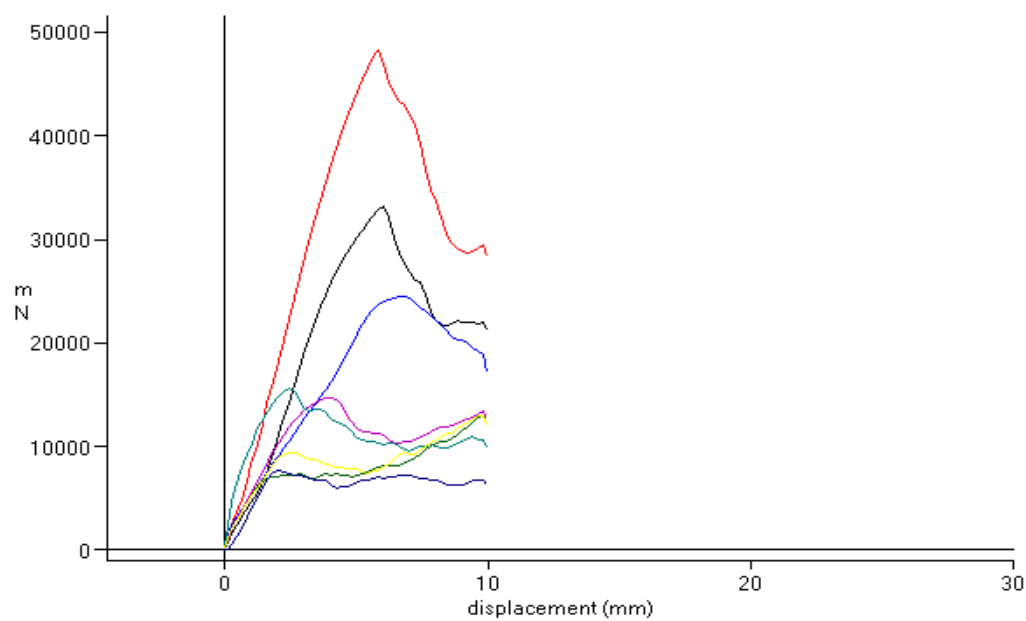
There was no significant difference found between the peaches grown under three different treatments with respect to their flesh firmness as shown in (Table 4). Figures 5, 6, and 7 show the variation of firmness in peaches from one harvest date (August 11, 2102) between the individual treatments. Firmness is inversely proportional to ripeness of the fruit; since there is no significant difference between the treatments (Table 4) all fruits were assumed to be equally ripened. However, many other factors contribute to ripeness like ethylene production, respiration, skin ground color and others.



*Figure 5.* Firmness of Conventional Peaches Harvested on 8-11-2012.



*Figure 6.* Firmness of Transitional Organic Peaches Harvested on 8-11-2012.



*Figure 7* Firmness of Organic Peaches Harvested on 8-11-2012.

Table 4

*Physical Parameters Data Between the Treatments*

Treatment	conventional	transitional	organic
equatorial diameter (mm)	86±4 <sup>a</sup>	82±4 <sup>b</sup>	80±5 <sup>b</sup>
top diameter (mm)	72±4 <sup>a</sup>	71±4 <sup>a</sup>	73±3 <sup>a</sup>
pit length (mm)	41±3 <sup>a</sup>	41±2 <sup>a</sup>	41±1 <sup>a</sup>
pit width (mm)	30±2 <sup>a</sup>	29±2 <sup>a</sup>	29±1 <sup>a</sup>
SSC (brix %)	10.9±0.9 <sup>a</sup>	11.3±0.8 <sup>a</sup>	11.3±0.9 <sup>a</sup>
L* (l)	64±4 <sup>a</sup>	62±6 <sup>a</sup>	61±5 <sup>a</sup>
a*(l)	14±4 <sup>a</sup>	15±6 <sup>a</sup>	7±3 <sup>b</sup>
b* (l)	36±4 <sup>a</sup>	33±5 <sup>a</sup>	34±4 <sup>a</sup>
Hue (l)	20±7 <sup>a</sup>	24±10 <sup>a</sup>	12±5 <sup>b</sup>
L*	41±4 <sup>a</sup>	40±3 <sup>a</sup>	40±4 <sup>a</sup>
a*	19±5 <sup>a</sup>	17±4 <sup>a</sup>	16±6 <sup>a</sup>
b*	14±3 <sup>a</sup>	12±2 <sup>a</sup>	12±3 <sup>a</sup>
Hue	36±5 <sup>a</sup>	39±5 <sup>a</sup>	39±8 <sup>a</sup>
TA % (g of malic acid per 100 ml juice)	0.97±0.08 <sup>a</sup>	0.80±0.07 <sup>b</sup>	1.04±0.11 <sup>c</sup>
SSC:TA	11.3±0.8 <sup>a</sup>	14.2±1.6 <sup>b</sup>	10.9±1.1 <sup>a</sup>
Firmness (mN)	25,000±13,000 <sup>a</sup>	19,000±12,000 <sup>a</sup>	21,000±14,000 <sup>a</sup>

Note: Values sharing similar letters within rows (*a*, *b*, and *c*) are not significantly different ( $p \geq 0.05$ )

\* Mean ± SEM

### **Sensory Evaluation of Peaches**

A 120-member consumer panel evaluated all three groups of peaches grown under different treatments. Degree of color liking of the conventionally grown fruits was significantly higher than the other two treatments (Table 5).

Overall liking of the peaches was higher for transitional organic fruits, followed by conventional fruits and then organically grown ( $p = 0.001$ ). Flavor liking was rated higher in transitional organic, followed by conventional and organic treatments respectively (Table 5). SSC: TA was significantly higher in transitionally grown fruits (Table 4) which might have affected the consumer's score in overall liking and flavor liking of fruits. There was no significant difference between the SSC: TA in conventionally and organically grown peaches but TA of the organic fruits were significantly higher than conventionally grown fruits since TA is the composition of organic acids which gives off flavors and negatively affect consumer scores; higher the ratio of SSC:TA indicates there was more sugar content and less TA which might have affected consumers give higher overall liking to transitional organic fruits.

Transitional organic peaches were rated significantly higher in juiciness ( $p = 0.0001$ ) than conventional and organic peaches. Sourness liking was given significantly higher score in transitional organic peaches ( $p = 0.0002$ ) than other two treatments. The texture of transitional organic peaches was preferred ( $p = 0.0001$ ) other two treatments.



Table 5

*Sensory Analysis of Peaches Treated with Different Treatments*

Attribute	Transitional			p - value
	Conventional	organic	Organic	
	<i>a</i>	<i>a</i>	<i>a</i>	
Smell Liking	7.1	6.86	6.84	0.0427
	<i>a</i>	<i>a</i>	<i>b</i>	
color liking	7.07	7.01	6.25	0.0001
	<i>b</i>	<i>a</i>	<i>c</i>	
overall liking	6.43	6.98	5.86	0.0001
	<i>b</i>	<i>a</i>	<i>c</i>	
flavor liking	6.29	6.95	5.87	0.0001
	<i>b</i>	<i>a</i>	<i>c</i>	
Juiciness liking	6.11	6.81	5.46	0.0001
	<i>b</i>	<i>a</i>	<i>b</i>	
Tartness/sourness liking	5.81	6.32	5.4	0.0002
	<i>b</i>	<i>a</i>	<i>b</i>	
texture/firmness liking	6.02	6.83	5.63	0.0001

Note: Values sharing similar letters within rows are not significantly different ( $p \geq 0.05$ ),

\* Means of the sensory scores by 120 panelists were given.

### Total Phenol Concentration

The total phenol concentration of the peaches is shown in Figure 8. The results indicate there were significantly lower concentrations of TP in conventionally grown fruits than the other two treatments (Figure 8).

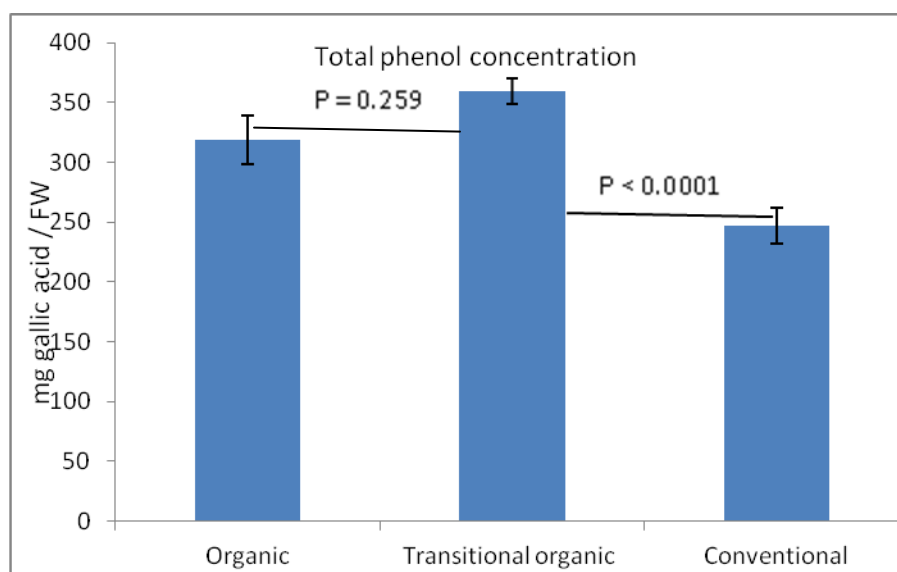


Figure 8 Total Phenol Concentration of the Treatments.

Biosynthesis of phenolic compounds in plants is strongly affected by the cultivator techniques (Häkkinen & Törrönen, 2000), environmental conditions and the fertilizers used. It has previously been reported that the phenol concentration is influenced by level of available nitrogen (Brandt & Molgaard, 2001). Increase in phenolic compounds is related to the defense role they play in plants under stressed conditions (Dixon & Paiva, 1995).

## HEAD SPACE SOLID PHASE MICRO-EXTRACTION GAS CHROMATOGRAPHY MASS SPECTROMETRY

The initial output from the HS-SPME-GC-MS analysis contained 79 potential compounds that were detected in the HS of the samples. This is similar to the average amount (75) of volatiles detected in previous studies (Sánchez et al., 2012 & Zhang & Pawliszyn, 2005) . Most of the volatile compounds detected fall under the categories of alcohols, aldehydes, ketones, lactones, esters, terpenoids, phenols and carboxylic acids. Table 6 shows those compounds that showed significant difference between the treatments along with CAS identification and the odor generally associated with each compound. Volatile data was normalized with internal standard 1, 2 di-chloro benzene and represented as the ratio to surrogate. Figure 9 shows the variation between the volatile compounds that showed significant difference.

Some volatiles are correlated with quality parameters which are responsible for a consumer acceptable, ripe peach (Jones et al., 2003). Volatile compounds showed strongest correlation with respect to equatorial diameter in conventional peaches (Table 7). Peach fruit quality is directly affected by the fruit maturity parameters (SSC, size, color, TA, and flesh firmness). The peel ground color change from green to orange-red is a common field method used to identify harvest-ready fruit to get better quality. This process corresponds to an increase in SSC content, increase in size, decrease in titratable acidity and flesh softening (Sánchez et al., 2012). Equatorial diameter in conventional fruits was strongly positively correlated to alpha-santalol ( $r = 0.645^{**}$ ) and also 7 other volatile compounds as shown in Table 13, suggesting that these volatiles increase during

of fruits. Myristic acid, methyl ester was highly negatively correlated with top diameter in organic peaches as shown in Table 8. In transitional organically grown peaches most of the lactones were seen to be positively correlated with the SSC whereas in organic peaches 3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran and linalyl alcohol were found to be highly negatively correlated with SSC. Lactones were seen to be highly negatively correlated with all the treatments (gamma-undecalactone was found highly negatively correlated to all the treatments  $r = -0.550^{**}$ ,  $-0.541^{**}$  and  $-0.518^*$  for conventional, transitional organic and organic treatments respectively) with respect to firmness (Table 9). The concentration of lactones increases during the maturity (Jones et al., 2003) and gamma- undecalactone which showed highly negative correlation to firmness in all treatments, also it had no significant difference of its concentration between the treatments which shows that all the fruits must have been equally ripened at the time of harvest and processing.

Eleven volatile compounds showed significant differences (Figure 9) between the treatments. 1-hexyl acetate, cis-3-hexenyl-1-acetate, n-heptanoic acid, ethylhexanoic acid, octanoic acid and nonanoic acid were found at significantly higher concentrations in conventional peaches than other two treatments. Tolualdehyde, myristic acid, methyl ester and pentadecanoic acid, methyl ester were found to be significantly higher in organic treatment, and propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester was found to significantly lower in concentration. Isomenthone and gamma-nonalactone were significantly higher in the transitional organic treatment. Interestingly, there was no significant difference between the treatments for smell liking in the sensory data (Table 5). Presence of a volatile compound that is relatively high doesn't infer that it

significantly contributes to flavor (Tieman et al., 2012). The synergistic and antagonistic interactions in complex food cannot be altered by concentration and odor threshold of an individual volatile (Tieman et al., 2012). 6-Pentyl-2H-pyran-2-one and isomenthane showed highly negatively correlated to TA in organic peaches ( $r = -0.689^*$ ,  $0.645^*$  respectively), organic peaches showed significantly higher in TA and Transitional organic peaches showed significantly lower in concentration of TA, isomenthane was found to be significantly higher in transitional organic peaches than other treatments; this shows that increase in concentration of isomenthane is lowering the TA in these fruits.

Table 6

*Volatiles with Significant Difference Between Treatments*

	CAS Number	Odor
1-Hexyl acetate	142-92-7	Fruity, green apple banana sweet
n-Heptanoic acid	111-14-8	Cheesy, waxy, sweaty, fermented, pineapple and fruity
Tolualdehyde	100-52-7	Almond, fruity, powdery, nutty and benzaldehyde
Octanoic Acid	124-07-2	fatty waxy, rancid, oily vegetable, cheesy
Nonanoic acid	112-05-0	Waxy, dirty and cheesy with a cultured dairy nuance
gamma.-Nonalactone	104-61-0	Sweet, creamy, coconut, fatty with oily buttery nuances
cis-3-Hexenyl-1-Acetate	1708-82- 3	green fruity banana apple
Ethylhexanoic acid	149-57-5	Faint specific odor
Isomenthone	491-07-6	Minty, cooling, sweet, peppermint-like.
Propanoic acid, 2-methyl- , 3-hydroxy-2,4,4 trimethylpentyl ester	74367- 34-3	sweet fruity pineapple spicy floral
Myristic acid, methyl ester	67762- 40-7	Honey, Fatty coconut, cognac odor

Odor description were taken from the website [www.thegoodscentscompany.com/](http://www.thegoodscentscompany.com/)

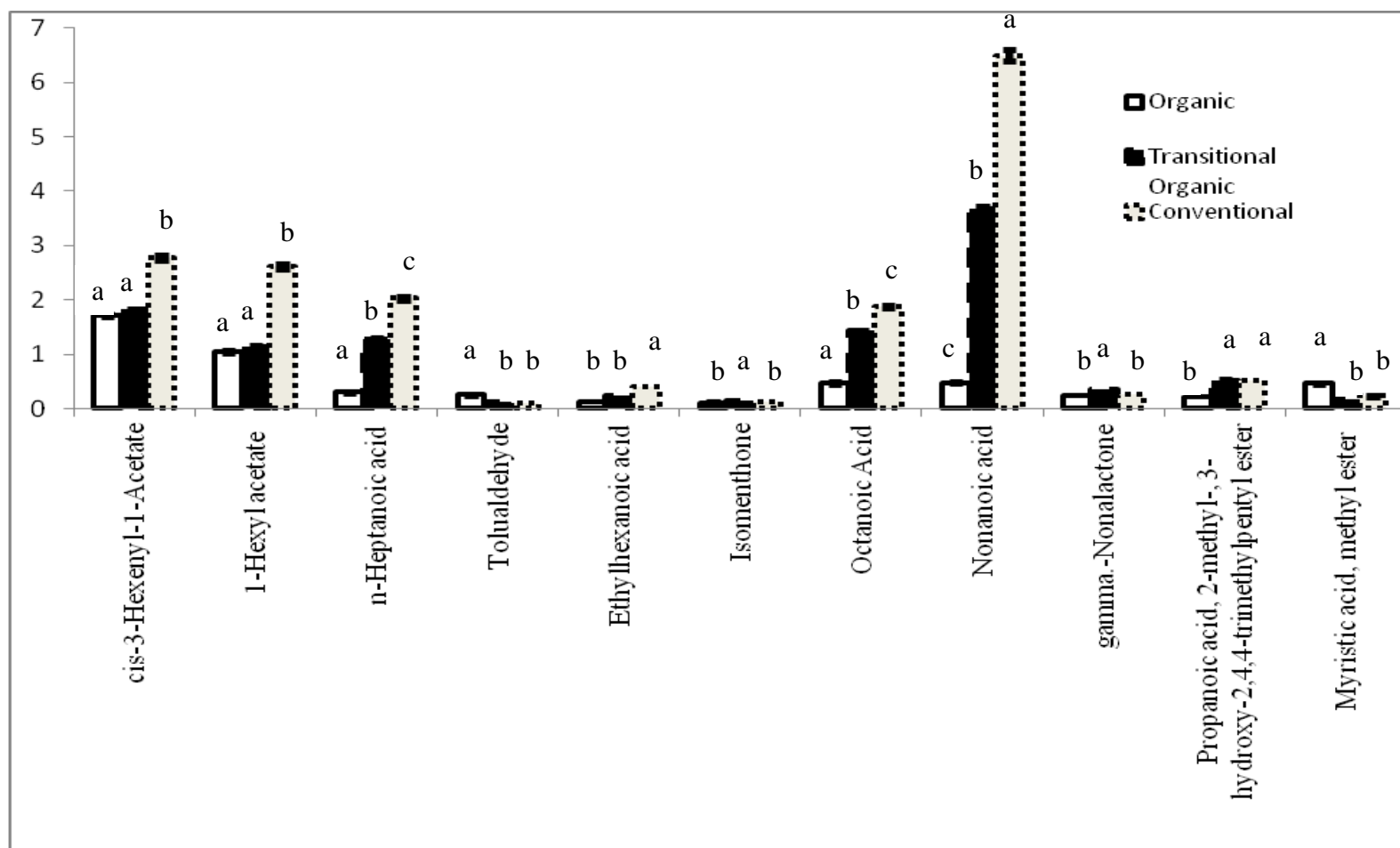


Figure 9. Ratio to surrogate of headspace volatile compounds that showed significant difference between the three treatments.

Table 7

*Correlation of Certain Aroma Volatiles with Equatorial Diameter*

Conventional	Equatorial diameter	Transitional organic	Equatorial diameter	Organic	Equatorial diameter
Alpha-santalol	.645**	No volatiles correlated		Ocimenol	.787**
Cyclopentyl cyclopentanone	.571**			2-(2- Ethylhexyloxy) ethanol	-.637*
n-Heptanoic-acid	.568**				
p-Menthatriene	.561**				
Isooctanol	.539**				
Gamma-Caprolactone	.531**				
Tridecyne	.516**				
Menthol	.513**				

\*\* Correlation is significant at the 0.01. \* Correlation is significant at the 0.05.



Table 8

*Correlation of Certain Aroma Volatiles with Top Diameter*

Conventional	Top diameter	Transitional	Top diameter	Organic	Top diameter
Tridecyne	.541 <sup>**</sup>	gamma-caprolactone	.558 <sup>**</sup>	Myristic acid, methyl ester	-.644 <sup>*</sup>
p-Menth-1-en-9- al	.468 <sup>*</sup>	Alpha-Santalol	.521 <sup>**</sup>		
Cyclopentylcyclo pentanone	.459 <sup>*</sup>	delta-undecalactone	.481 <sup>**</sup>		
p-Menthatriene	.454 <sup>*</sup>	Octanol	.473 <sup>**</sup>		

<sup>\*\*</sup> Correlation is significant at the 0.01. <sup>\*</sup> Correlation is significant at the 0.05.

Table 9

*Correlation of Certain Aroma Volatiles with Firmness*

Conventional	Firmness	Transitional	Firmness	Organic	Firmness
gamma-undecalactone	-.550 <sup>**</sup>	p-menth-1-en-8-ol	.524 <sup>**</sup>	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	.461 <sup>*</sup>
delta-undecalactone	-.505 <sup>**</sup>	Linalyl alcohol	.515 <sup>**</sup>	1,3,8-p-Menthatriene	.453 <sup>*</sup>
delta-decalactone	-.407 <sup>*</sup>	Cis-3-Hexenyl-1-acetate	.474 <sup>**</sup>	Acetic acid, octyl ester	-.510 <sup>*</sup>
Chloroacetic-acid-dodec-9-ynyl-ester	-.400 <sup>*</sup>	Ocimenol	.450 <sup>**</sup>	Gamma-Undecalactone	-.518 <sup>*</sup>
		gamma-undecalactone	-.541 <sup>**</sup>	delta-undecalactone	-.551 <sup>*</sup>
		delta-undecalactone	-.539 <sup>**</sup>	2-Hexen-1-ol acetate	-.553 <sup>*</sup>

<sup>\*\*</sup> Correlation is significant at the 0.01. <sup>\*</sup> Correlation is significant at the 0.05.

Table 9

*Correlation of Certain Aroma Volatiles with Titratable Acidity*

Conventional	TA	Transitional organic	TA	Organic	TA
Tridecyne	.671 <sup>**</sup>	Ocimenol	.396 <sup>**</sup>	6-Pentyl-2H-pyran-2-one	-.689 <sup>*</sup>
p-Cymen-8-ol	.630 <sup>**</sup>	p-menth-1-en-8-ol	.368 <sup>*</sup>	Isomenthone	-.645 <sup>*</sup>
Nonanoic-acid	.626 <sup>**</sup>	Dihydro-4-methyl-2-2-methyl-1-propenyl-2H-pyran	.336 <sup>*</sup>		
n-heptanoic-acid	.596 <sup>**</sup>	delta-decalactone	-.337 <sup>*</sup>		
Octanoic-acid	.596 <sup>**</sup>	gamma-undecalactone	-.321 <sup>*</sup>		
Ethylhexanoic-acid	.553 <sup>**</sup>	delta-undecalactone	-.315 <sup>*</sup>		
Menthol	.537 <sup>**</sup>				
Alpha-santalol	.510 <sup>**</sup>				
Isooctanol	.508 <sup>**</sup>				

\*\* Correlation is significant at the 0.01. \* Correlation is significant at the 0.05.

### Headspace Principal Component Analysis

Using the 11 compounds that showed a significant difference between treatments, Table 12 PCA was performed. The eigen values of the correlation matrix in Table 11 were used to determine that the first three principal components were sufficient to explain 74.17% of the variation in the data.

Table 10

*Eigenvalues of the Correlation Matrix for the Headspace Principal Component Analysis*

	Eigenvalue	Variability (%)	Cumulative %
F1	5.079	46.168	46.168
F2	1.735	15.773	61.942
F3	1.346	12.236	74.178
F4	0.991	9.009	83.186
F5	0.697	6.334	89.521
F6	0.510	4.635	94.156
F7	0.328	2.978	97.134
F8	0.135	1.229	98.363
F9	0.078	0.712	99.075
F10	0.065	0.592	99.667
F11	0.037	0.333	100.000

Table 11

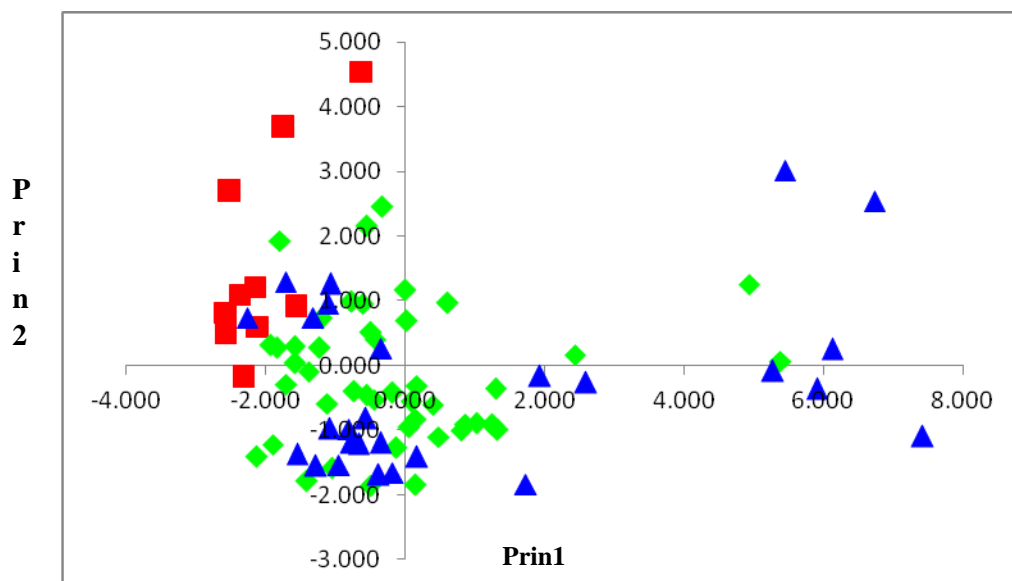
*Eigenvectors of Principal Component 1, Principal Component 2, and Principal Component 3 for the Headspace Principal Component Analysis*

	Prin1	Prin2	Prin3
cis-3-Hexenyl-1-Acetate	0.238	0.243	-0.499
1-Hexyl acetate	0.316	0.261	-0.420
n-Heptanoic acid	0.415	-0.096	-0.017
Tolualdehyde	0.026	0.513	0.188
Ethylhexanoic acid	0.412	-0.003	-0.010
Isomenthone	0.270	0.240	0.363
Octanoic Acid	0.408	-0.180	0.067
Nonanoic acid	0.396	-0.209	-0.047
gamma.-Nonalactone	0.151	0.272	0.583
Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	0.286	-0.193	0.215
Myristic acid, methyl ester	-0.013	0.596	-0.116

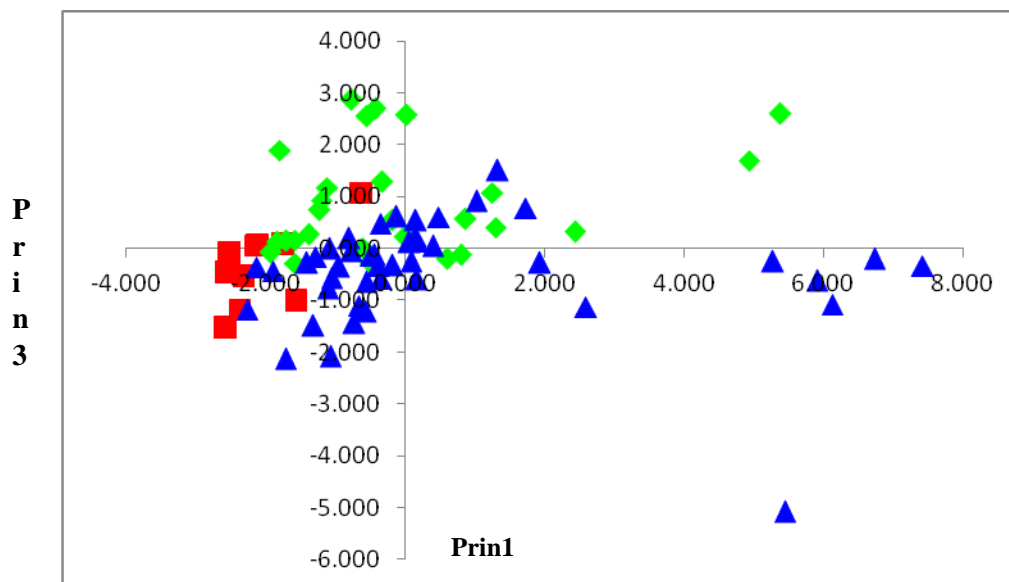
Using 0.3 as a cut off for the eigen vectors (Table 12), 1-Hexyl acetate, n-Heptanoic acid, Ethylhexanoic, Octanoic Acid, and Nonanoic acid play the largest role in separating the treatments. The eigenvectors from the same table for Prin2 indicate that Tolualdehyde and Myristic acid, methyl ester play the largest role in separating between the treatments. The eigenvectors from Prin3 indicate that cis-3-Hexenyl-1-Acetate, 1-

Hexyl acetate, Isomenthone, and gamma.-Nonalactone play most of the role in separating between the treatments.

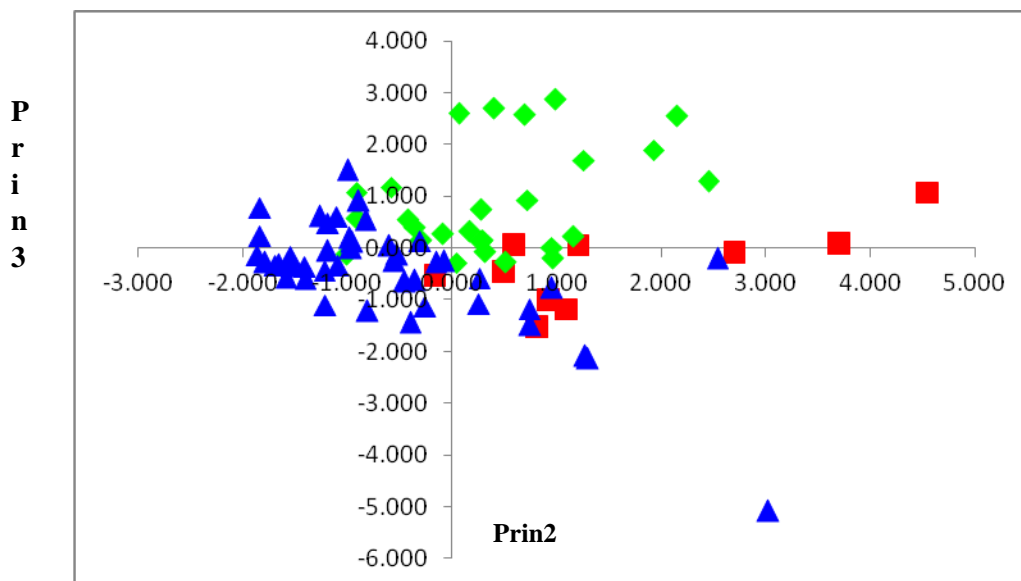
Figure 10 showed some discrimination between the treatments, as transitional organic replicates were seen mostly clustered on the negative side of PC2 over PC1 which was influenced by Tolualdehyde and Myristic acid, methyl ester. Although, there is no significant difference between the smell likings for the treatments (Table 5) conventional fruits had higher rating to smell liking. Conventional treatment replicates showed more clustering on the positive side of the PC3 (Figure 11 and 12) which is influenced by cis-3-Hexenyl-1-Acetate, 1-Hexyl acetate, Isomenthone, and gamma.-Nonalactone. All these volatiles influencing PC3 give a fruity and fresh odor, which might have made consumers give a higher rating to the conventional peaches (Table 5).



*Figure 10.* Score plot for headspace principal component analysis (PC1 and PC2); square: organic, triangle: transitional organic, polygon: conventional.



*Figure 11.* Score plot for headspace principal component analysis (PC1 and PC3); square: organic, triangle: transitional organic, polygon: conventional.



*Figure 12* Score plot for headspace principal component analysis (PC2 and PC3); square: organic, triangle: transitional organic, polygon: conventional.

### Metabolomics Analysis

The metabolite analysis of peaches produced 49 and many of them are sugars, sugar alcohols and organic acids compounds. This is somewhat lower than the average identified metabolites 58 in previous studies (Roessner-Tunali et al., 2003 & Lombardo et al., 2011). Seven metabolites showed significant difference between treatments on a one way ANOVA as a function of treatment (Table 13).

Most of the metabolites that showed differences between the treatments were organic acids. Organic peaches were significantly higher in all the organic acids except lactic acid. In ripe peaches major soluble acids are malic acid and citric acid.

Table 12

*One way ANOVA for Metabolites with Treatment as a Function*

Metabolites	Conventional (Ratio of surrogate/gm of fruit weight)	Transitional Organic (Ratio of surrogate/gm of fruit weight)	Organic (Ratio of surrogate /gm of fruit weight)	<i>p</i> -value
Lactic acid	$0.13 \pm 0.07^a$	$0.05 \pm 0.01^b$	$0.04 \pm 0.01^b$	0.037
D-malic acid	$7 \pm 3^a$	$13 \pm 6^a$	$50 \pm 30^b$	0.01
Succinic acid	$0.1 \pm 0.1^b$	$0.1 \pm 0.1^b$	$0.3 \pm 0.1^b$	0.01
Citric acid	$0.2 \pm 0.1^b$	$3 \pm 1^b$	$14 \pm 9^b$	0.01
D-Mannopyranose	$15 \pm 4^b$	$22 \pm 5^{ab}$	$40 \pm 20^a$	0.05
D-Fructofuranose	$10 \pm 2^a$	$8 \pm 3^a$	$43 \pm 30^b$	0.01
Quinic acid	$4 \pm 2^b$	$4 \pm 1^b$	$20 \pm 10^b$	0.01

\* Values sharing similar letters (within rows) are not significantly different ( $p \geq 0.05$ ),

\* Mean  $\pm$  SEM



Table 20 shows that the two major acids were found higher in concentrations in organic peaches. This might have affected the consumer acceptability, as organic peaches were least preferred (Table 5). This agrees with Malundo et al., who concluded that fruits with higher acid content can have negative effect on consumer acceptability of fruits.

Table 14 shows the variation in the predominant sugars found in the treatments. Although organic peaches showed somewhat higher concentrations of sugars, it was not significantly higher than other treatments.

Table 13

*Predominant Sugars Variation in the Treatments*

	organic	conventional	transitional organic	<i>p</i> -value
Sucrose	91 ± 57 <sup>a</sup>	54 ± 32 <sup>a</sup>	49 ± 25 <sup>a</sup>	0.167
Fructose	105 ± 60 <sup>a</sup>	56 ± 26 <sup>a</sup>	57 ± 30 <sup>a</sup>	0.080
d-Glucose	63 ± 40 <sup>a</sup>	55 ± 26 <sup>a</sup>	32 ± 21 <sup>a</sup>	0.067

\* Values sharing similar letters within rows (a, b, and c) are not significantly different ( $p \geq 0.05$ )

\* Mean ± SEM

## CONCLUSIONS

From this study we can conclude farm management techniques can affect the overall quality of peach fruit. Transitional organic peaches which were nitrogen stressed, developed more sweetness and significantly less titratable acidity; whereas conventionally grown peaches were bigger in size due to the increased availability of N as  $\text{NO}_3^-$  nitrate levels. Sensory data supported these results as the overall liking for transitional organic peaches (higher SSC: TA than other treatments) was significantly higher than conventional and organic peaches. Organic peaches were least liked by the consumers, which may be due to the high TA in these peaches. Total phenol concentration was found to be significantly lower in conventionally grown fruits compared to organic and a transitional organic fruit, as the bioavailability of N to these treatments is likely lower than conventional. There was no significant difference in firmness, which is related to the ripeness of the fruits. At this point there was no clear evidence on the equal ripeness in fruits which plays an important role in TA and consumer acceptability. Further studies may include measuring ripeness of fruit, respiration and ethylene production rates to get a bigger picture of the nutritional and physiological changes in fruits with respect to their farm management technique.

There was a significant difference between some volatiles that might contribute to the smell liking of the peaches. The HS SPME PCA provided a separation of the conventional treatment on PC3. The compounds that were most responsible for the variation are cis-3-Hexenyl-1-Acetate, 1-Hexyl acetate, Isomenthone, and gamma.-Nonalactone.

Organic treatment showed high concentrations of predominant acids in peaches which inversely affect the consumer acceptability. Organic peaches have more concentration of sugars but these were not significantly higher and variance in the sample size might some time effect the overall data. Transitional organic peaches were more liked and organic were least liked, but the nutritional values organic peaches bring can be the point of interest for the consumers. Future studies can be performed selecting less variance in the sample size.

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## **APPENDIX**



Table A 14

*One-way ANOVA for Equatorial Diameter*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Conventional vs Transitional organic	3.215	2.978	2.389	0.011	Yes
Conventional vs Organic	6.137	3.738	2.389	0.001	Yes
Transitional organic vs Organic	2.922	1.885	2.389	0.150	No

Table A 2

*One-way ANOVA for Top Diameter as a Function of Treatment*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Organic vs Conventional	1.259	0.871	2.389	0.660	No
Organic vs Transitional organic	1.971	1.444	2.389	0.324	No
Conventional vs Transitional organic	0.711	0.748	2.389	0.735	No

Table A3

*One-way ANOVA for Soluble Solid Content as a Function of Treatment*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Transitional organic vs Organic	0.043	0.146	2.389	0.988	No
Transitional organic vs Conventional	0.422	2.043	2.389	0.109	No
Organic vs Conventional	0.379	1.206	2.389	0.453	No

Table A4

*One-way ANOVA for Titratable Acidity as a Function of Treatment*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Organic vs Conventional	0.077	2.391	2.389	0.050	Yes
Organic vs Transitional organic	0.240	7.902	2.389	< 0.0001	Yes
Conventional vs Transitional organic	0.163	7.712	2.389	< 0.0001	Yes

Table A5

*One-way ANOVA for Firmness as a Function of Treatment*

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Conventional vs Organic	3547.054	0.737	2.389	0.742	No
Conventional vs Transitional organic	6152.415	1.944	2.389	0.133	No
Organic vs Transitional organic	2605.361	0.573	2.389	0.835	No

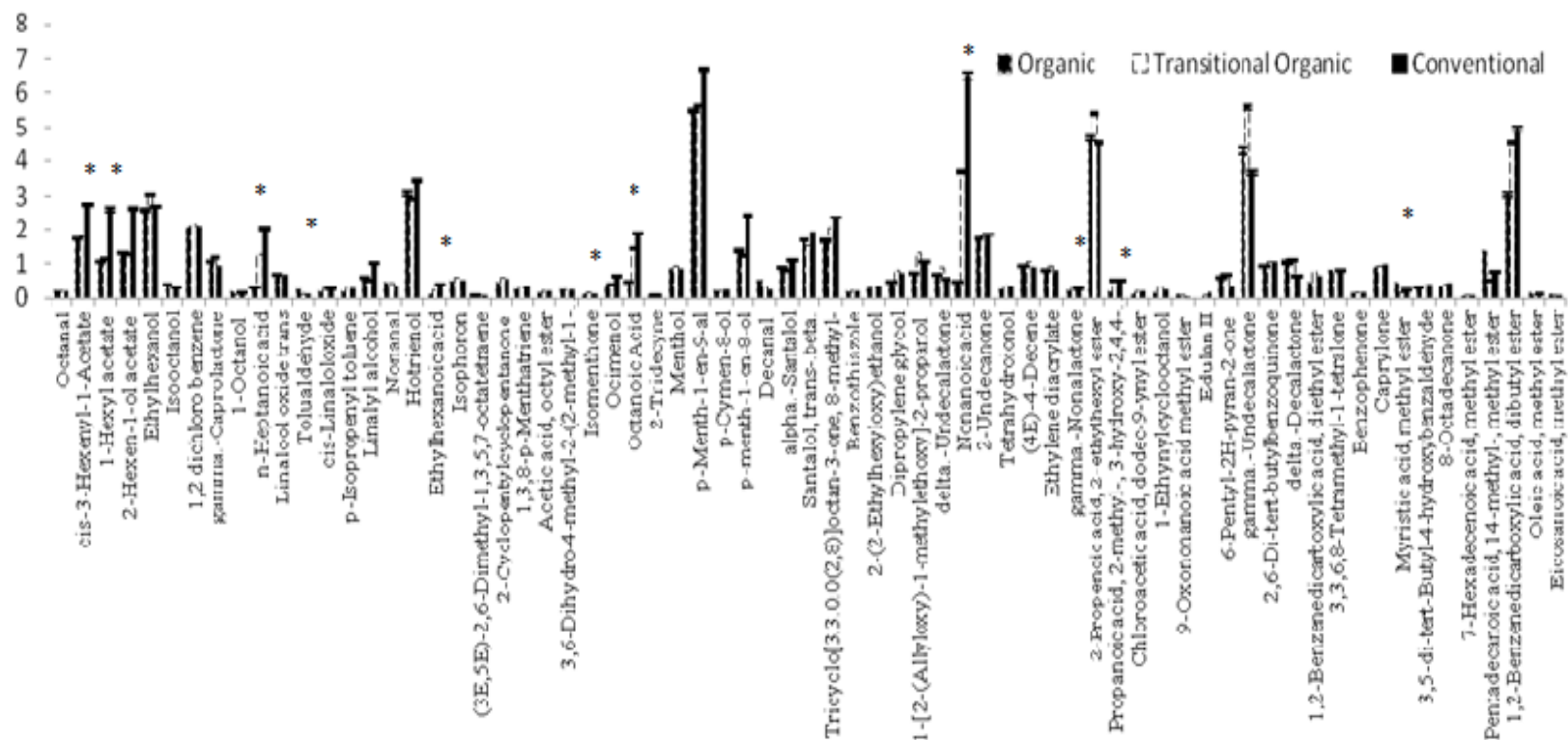


Figure A1 Ratio to surrogate of headspace volatile compounds from peach samples of the three treatments. \* = Ratio to surrogate is significantly different between treatments ( $p \leq 0.05$ ).